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SATELLITE RADIANCE DATA ASSIMILATION: CODE MIGRATION TO SCALABLE ARCHITECTURES

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14. ABSTRACT
We developed a highly scalable version of the MM5 4d-Var application. The application consists of a meteorological analysis code that provides accurate depictions of the state of the atmosphere, has been applied successfully to a large number of cases, and the results have been documented in peer reviewed forums. Prior to this project, this code was optimized for vector computer architectures. By rewriting this code in order to make it "scale" (i.e., performance increases linearly) as additional CPUs are devoted to the calculations, significant speedups were achieved on the class of computers referred to as Massively Parallel Processors. The 4d-Var technique performs a series of iterations and requires computational power measured in the tens of gigaflops for real-time application. Proven strategies and techniques were employed to develop the scaleable version of this code and to attain the objective performance metrics. Among the coding strategies employed was domain decomposition. A tested, scalable 4d-Var code was delivered, along with user documentation. During the later half of this contract, we investigated the potential impact of optical turbulence data on upper-air data analysis. The task involved the development of additional software for the MM5 4d-Var code and applying it to C_n^2 data obtained by AFRL. The preliminary results from that exercise suggest that C_n^2 data have the potential to improve upper-atmospheric analyses and the NWP model forecasts made from

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1. SUMMARY

In the spring of 2000, Atmospheric and Environmental Research , Inc. (AER) was awarded a contract by the Air Force Research Laboratory for a proposal submitted under the Broad Agency Announcement to conduct research and development work. AER's contribution to this effort would be performed as a team member in a Department of Defense (DoD) High Performance Computing and Modernization Office (HPCMO) project aimed at improving the quality and usefulness of weather forecast data in support of the USAF mission. The armed forces currently devote a large amount of resources to the timely collection and dissemination of weather information to minimize negative weather impacts on the warfighter and to use weather knowledge as a force multiplier. A core activity at military weather centers involves the use of analysis and forecast models. The quality of the products produced by these analysis and forecast models is highly dependent upon the conventional observing network (e.g., radiosondes and surface observing stations). However, this network is not capable of sampling the atmosphere with the needed temporal and spatial resolution to accurately resolve the theater-scale weather patterns of interest. While *remotely* measured weather data have the potential to overcome this deficiency, its use in theater-scale models is problematic. Among the difficulties is the fact that the remotely measured quantity must first be converted into one of the model's native dependent variables—often with a loss of accuracy. The four-dimensional variational (4d-Var) approach can be used to overcome this difficulty since it can directly assimilate any measured quantity. However, the computational demands of this approach far exceed the compute cycles available at the typical weather center. During this project, we developed a highly scalable version of a 4d-Var application that has the potential to execute within the time constraints of an operational center. Its contribution to the objectives of dominant battlespace awareness and information superiority espoused in Joint Vision 2010 can be considerable. It seeks to more fully exploit vital space-based environmental monitoring assets to improve situational awareness, mission planning, and weapon system execution. The application developed under this project is state-of-the-art, consists of a meteorological analysis code that provides accurate depictions of the state of the atmosphere, has been applied successfully to a large number of cases, and the results have been documented in peer reviewed forums. Before this project, this code was optimized for vector computer architectures. By reengineering this code to make it "scale" (i.e., performance increases linearly) as additional CPUs are devoted to the calculations, significant speedups were achieved on the class of computers referred to as Massively Parallel Processors (MPP). The 4d-Var technique performs a series of iterations that require computational power measured in the tens of gigaflops for real-time application. Proven strategies and techniques were employed to develop the scaleable version of this code. Among the coding strategies employed was domain decomposition. The project reached all of its critical test goals, which included tests for scalability, portability, and correctness. Test results were confirmed by NCAR. For scalability, the wall clock time of the scalable MM5v3 4d-Var was reduced by factors of up to 36 times (speedup was case dependent) from that of the baseline on 64 nodes of an IBM SP P3 system, and by factors of up to 196 times on 64 nodes of a Compaq ES-45 system. Correctness was measured by comparison with the MM5v1 4d-Var code on a single processor, and was found to differ by less than 3.5

percent. Correctness was also measured in terms of differences between multiprocessor and single processor runs, where differences were less than 1 percent. A tested, scalable 4d-Var code was delivered, along with periodic progress reports, and full user documentation. During the later half of this contract, we investigated the potential impact of optical turbulence data on upper-air data analysis. The task involved developing additional software for the MM5 4d-Var code and applying it to C_n^2 data obtained by AFRL. The preliminary results from that exercise suggest that C_n^2 data have the potential to improve upper-atmospheric analyses and the NWP model forecasts made from them.

2. INTRODUCTION

This section provides some background and introductory material. The subsequent sections present a summary of the activities conducted for this project. In section 3 we will present the methods and procedures used to develop, test, and evaluate the scalable MM5v3 4d-Var code. Section 3.11 includes the work on the optical turbulence task. Section 4 contains test results and discussion. Concluding remarks are presented in Section 5.

2.1 DoD High Performance Computing Modernization Office

The Office of the Secretary of Defense is investing significant resources in high performance computing to provide the United States military with a technological advantage to support warfighting requirements. The High Performance Computing Modernization Program (HPCMP; http://www.hpcmo.hpc.mil) provides advanced hardware, computing tools and training to DoD researchers utilizing the latest technology to aid their mission in support of the warfighter. The program has three initiatives:

(1) High performance computing centers which consist of major shared resource centers (MSRCs) and distributed centers (DCs),

(2) The Defense Research and Engineering Network (DREN),

(3) The Common High Performance Computing Software Support Initiative (CHSSI).

CHSSI will next be described in more detail.

2.1.1 Common High Performance Computing Software Support Initiative

CHSSI is an application software development component of the HPCMP that provides DoD research scientists and engineers with technical codes that exploit scalable computing systems. The CHSSI applications are selected based on their critical need. These products facilitate a large fraction of the DoD science and technology and developmental test and evaluation computational workload in support of DoD warfighting requirements.

In January 1999, the Air Force Research Laboratory teamed with Atmospheric and Environmental Research, Inc. (AER), Florida State University (FSU), and the National Center for Atmospheric Research (NCAR) and submitted a proposal to create a version of

the MM5 4d-Var analysis application (see below) that scales on a class of computers known as Massively Parallel Processors (MPP). This software would enable its users to achieve runtime efficiencies that would make possible operational implementation of the 4d-Var technique. In November 1999, the HPCMP Office informed the team that the proposal was accepted, and work began in February 2000. The project was the fifth selected under the Climate/Weather/Ocean Computational Technical Area (CTA) of CHSSI, and is identified as CWO-5.

2.2 DoD Weather

DoD operates a military environmental service system to provide specialized worldwide meteorological, space environmental, and oceanographic analysis and prediction services in support of military forces. This system directly supports all phases of military operations, from strategic planning to tactical operations. While the Army and Marine Corps each have a small, specialized weather support capability, the Naval Meteorology and Oceanography Command and Air Force Weather are the primary sources of military weather products. The military weather services contribute to the national and international weather observing capability by taking conventional observations on land and at sea where there are no other conventional weather observing capabilities and where the observations are most needed to meet military requirements. In addition, DoD maintains specialized observing capabilities, such as the Defense Meteorological Satellite and Global Weather Intercept Programs, to meet unique military requirements. Observational data are sent by military communications networks to military and civil facilities in the United States and overseas.

2.2.1 Air Force Weather Agency

The Air Force Weather Agency (AFWA) is a field operating agency that reports to HQ USAF/XOW, the Deputy Chief of Staff for Air and Space Operations. AFWA provides strategic-level weather support (global and synoptic scale) for their worldwide customers, and fulfills other unique mission requirements. AFWA is the primary production center for providing weather analyses and forecasts for Air Force and Army operations. Worldwide weather data are relayed to AFWA and blended with civil and military meteorological satellite data to construct a real-time, integrated environmental database. Computer programs digest the data and process it with models of the atmosphere to forecast its future behavior.

Our primary intended customer for this project is the AFWA. During the course of this project, we considered the present AFWA operating environment and likely future capabilities and factor them into the software development process. An example of this would be the choice of a computer platform on which to run the 4d-Var code; we selected an IBM SP-class of computer since this is the type of system presently in use at AFWA. We also assumed that AFWA's computational facilities would keep pace with trends in the computing world, where CPU processing speeds are doubling approximately every 18 months. This would enable AFWA to implement 4d-Var, or some other variational method into operations in the 2005 time frame.

2.3 AFRL CHSSI Project

This section provides information on the CHSSI CWO-5 team, the Statement of Work defining AER's role in the CWO-5 project, the migration of the 4d-Var code to version 3 of the MM5, some relevant distributed memory (DM) issues, and the funding mechanism.

2.3.1 CHSSI Project Team

The project team for the CHSSI CWO-5 project is shown in Table 1.

Table 1. CHSSI CWO-5 project team and basic responsibilities

Name	Responsibilities
Dr. Frank Ruggiero AFRL/VSBYA	Project Leader, overall project management, interface to HPCMO, coordination of efforts of various project members, writing scalable code, and post grant software maintenance
Dr. Thomas Nehrkorn Atmospheric Environmental Research	Meteorologist/Programmer, writing, testing scalable code; support reviews, code releases; maintain software repository
Mr. George Modica Atmospheric Environmental Research	Meteorologist/Programmer, writing, testing scalable code; support reviews, code releases, documentation; maintain document repository
Mr. Ernesto Sendoya Atmospheric Environmental Research	Software Engineer, software design, documentation, and review; monitor adherence to software engineering standards
Dr. Xiaolei Zou Florida State University	4d-Var Expert, responsible for conducting baseline test of the original 4d-Var software; development of incremental driver, bogus-data vortex assimilation codes
Mr. John Michalakes National Center for Atmospheric Research	Software Engineer/Programmer, manage code parallelization strategy and implementation, test and evaluation

The management structure of this project is illustrated in Figure 1. AFRL served as the overall program manager and interface to the HPCMO, with Florida St. University (X. Zou) and NCAR (J. Michalakes) providing technical management of the 4d-Var code. AER was responsible for software engineering activities, including code development, testing, and documentation. AER also supported reviews and provided software and document releases. While all three parties participated in different aspects of software development, AER played the coordinating role.

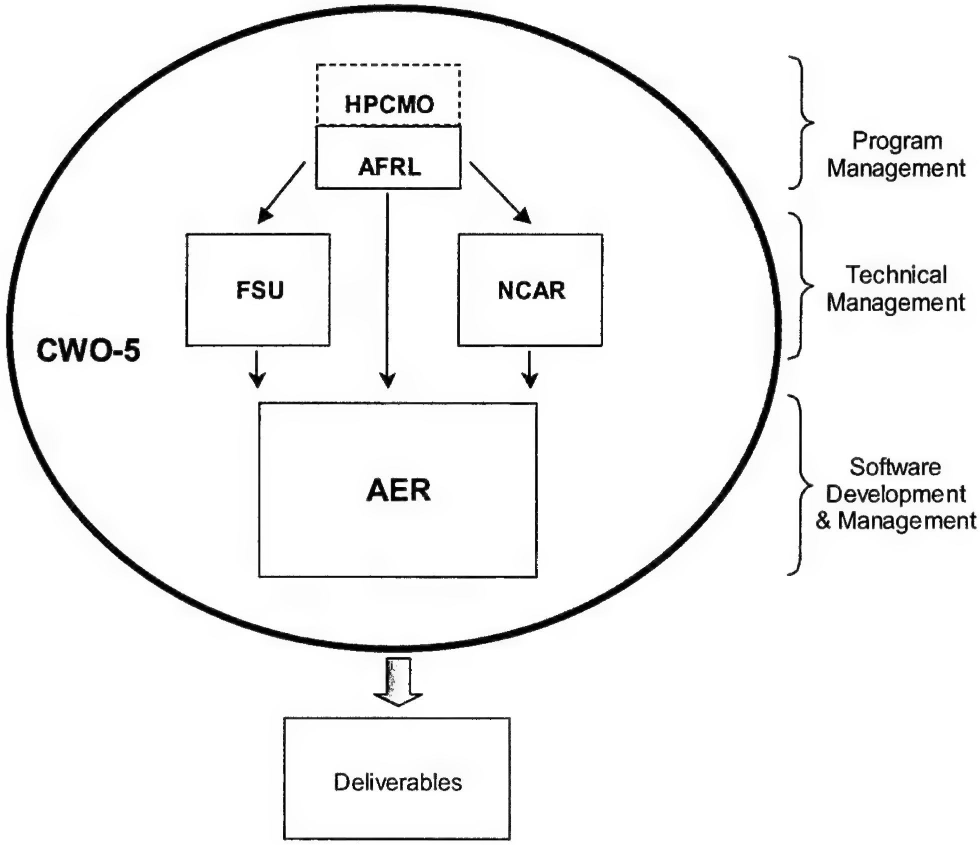

Figure 1. Illustration of the Management Structure Employed for CWO-5.

2.3.2 Variational Method

The variational method solves a minimization problem, in which a model initial state $\mathbf{x}(t_0)$ is found which minimizes an objective function. In meteorological applications, the cost function often takes a form similar to the following (see also, for example, Ide *et al.* 1997):

$$J[\mathbf{x}(t_0)] = \frac{1}{2}[\mathbf{x}(t_0) - \mathbf{x}^b(t_0)]^T \mathbf{B}_0^{-1}[\mathbf{x}(t_0) - \mathbf{x}^b(t_0)] + \frac{1}{2}\sum_{i=0}^{n}(\mathbf{y}_i - \mathbf{y}_i^o)^T \mathbf{R}_i^{-1}(\mathbf{y}_i - \mathbf{y}_i^o), \quad (1)$$

where $\mathbf{x}^b$ is the *a priori* background field with assumed error covariance $\mathbf{B}_0$, and $\mathbf{y}_i^o$ denotes the vector of observations at time t_i, and $\mathbf{R}_i$ is the corresponding observation error covariance matrix. The simulated observations $\mathbf{y}_i$ are obtained by applying the [in general, nonlinear] observation operator to the model predicted variables: $\mathbf{y}_i = H[\mathbf{x}(t_i)]$. The minimization is performed over an analysis time window $[t_o, t_n]$.

The 3d-Var algorithm can formally be written in the same way, except that the sum over *i* in the second RHS term in (1) is replaced by a single term; that is, only the observations at time t_o are considered in the minimization. In practice, observations within a data

cutoff window around t_o are grouped together for the nominal analysis time, and the background field is interpolated in time and space to the observation location and time.

Minimization of the variational analysis problem requires an estimate of the gradient of J with respect to the solution vector $\mathbf{x}(t_0)$, which is most efficiently computed with the adjoint of the observation operator (and, for 4d-Var, the adjoint of the forecast model). The MM5 4d-Var system is described in Section 2.3.3.

2.3.3 MM5 4d-Var System

During a three-year period ending in 1997, the Microscale and Mesoscale Meteorology Group at the National Center for Atmospheric Research (NCAR)—under the support of the National Science Foundation, the Federal Aviation Administration, and the Department of Energy—developed a mesoscale data assimilation system based on the nonhydrostatic version of MM5 and its adjoint (Zou et al. 1998). The initial version of the MM5 4d-Var system was coded for single processor computer architectures and its nonlinear, tangent-linear, and adjoint components were based on Version 1 of the MM5 (MM5v1). The MM5v1 4d-Var system included a bulk aerodynamic formulation of the planetary boundary layer, a dry convective adjustment, grid-resolvable large-scale precipitation and a Kuo-type cumulus parameterization in addition to the model dynamics. The MM5v1 4d-Var has since been updated to include the Grell cumulus parameterization, Dudhia's explicit moisture scheme, and a radiative upper boundary condition. The latest version also has the capability to use 8-byte MM5v2 input files as well as standard MM5v3 input files and to resume minimization from a restore file. The MM5v1 4d-Var can operate on multiple platforms, such as the DEC (Compaq) Alpha, SGI, and PC-Linux.

The background error covariance $\mathbf{B}_0$ in (1) is used to weight errors in the features of the background field relative to the observations. The assimilation system will assign less weight to those structures with large error relative to more accurately known background features and observations. Evaluation of $\mathbf{B}_0$ requires the inverse of the background error covariance matrix. With the length of the model state vector being on the order of 10^6, direct evaluation and storage of this matrix is computationally prohibitive. There are a number of different procedures to make the background weighting problem more tractable. The approach taken in the MM5v1 4d-Var system is to assume $\mathbf{B}_0$ is approximately diagonal in full-field space. A more elegant approach is taken e.g., in the WRF 3d-Var data assimilation through the introduction of a variable transformation, $\delta\mathbf{w} = \mathbf{Uv}$, so that the background error covariance matrix is approximately diagonal in $\mathbf{v}$ space. With proper normalization of $\mathbf{U}$, the background error covariance matrix can then be approximated by the identity matrix. This method has been used successfully in NCEP's spectral statistical interpolation (SSI) scheme (where the spectral modes are assumed to have uncorrelated error); similar approaches are in use at the ECMWF, and the mesoscale 3d-Var system developed at NCAR.

In general, the error structures represented by the background error covariance matrix are flow dependent and change from day to day depending on the synoptic regime and other factors. However, providing background "errors of the day" can be a costly endeavor, and is not easily implemented in practice. One way of approximating the

background error covariance data is with the "NMC-method" (Parrish and Derber 1992). In this method the background errors are approximated from averaged forecast differences, e.g.,

$$\mathbf{B} = \overline{\left(\mathbf{x}^b - \mathbf{x}^t\right)\left(\mathbf{x}^b - \mathbf{x}^t\right)^{\mathrm{T}}} = \varepsilon_b \varepsilon_b^{\mathrm{T}} \approx \overline{\left(\mathbf{x}^{T+24} - \mathbf{x}^{T+12}\right)\left(\mathbf{x}^{T+24} - \mathbf{x}^{T+12}\right)^{\mathrm{T}}}, \qquad (2)$$

where $\mathbf{x}^b$ is the background field, $\mathbf{x}^t$ is the true atmospheric state, and ε_b is the background error. The overbar in (2) represents an average in time and/or space. The WRF 3d-Var includes tunable background error files that were computed for a variety of horizontal spatial resolutions and for the major seasons of the year. The MM5v1 4d-Var application only has the option to use "direct observations," which consists of gridded analysis fields.

2.3.4 Statement of Work

The technical implementation plan, or statement of work (SOW) for this contract, concentrated on the development, validation, and demonstration of a scalable system for the 4d-Var data analysis of satellite radiance data. An overarching goal for CWO-5 was to develop an analysis system that achieves speed-up in wall-clock time sufficient to make feasible its use in an operational weather analysis and forecast center. To meet this operational requirement, we set an objective for the baseline system to achieve a wall-clock time speedup of 32 to 64 times that of the current version. While the 4d-Var system was designed to run on as many platforms as possible, development was focused on those platforms commonly available to potential users of the system such as AFWA and others in the operational and research communities, both inside and outside DoD. The analysis system, which uses a NWP model to constrain the analyzed state, includes physics parameterizations that are consistent with current mesoscale NWP models.

The MM5v1 version of the 4d-Var system runs on a vector-class machine using the non-hydrostatic form of the governing equations and simple physics parameterizations. The programming strategy followed an incremental series of four builds: The first build provided the candidate baseline code for the Software Acceptance Test (SAT). This build was comprised of, in essence, the NCAR MM5v1 4d-Var code (see 2.3.3) but ported to run on a single node of a MPP machine. The second build, the Alpha Test Code, included scalable non-linear and tangent-linear models, or NLM and TLM, respectively. The Beta Test Code, or third build, completed the development of the scalable 4d-Var system by including a scalable adjoint model (ADJ) system. The Beta build included radiosonde, surface, and satellite observation operators that would permit the use of those observations. The final build was the Initial Operation Capability (IOC) build. The IOC version implements the incremental driver and bogus data vortex assimilation options. All problems encountered during the extensive beta testing are corrected and incorporated into the IOC build, and any additional physics upgrades have been added as options to the system at this time. While the IOC code was not subject to review, it was prepared with the same software management methodology as in other releases.

The Work Breakdown Structure (WBS) provides the backbone of the development path for the CWO-5 code, and is included in the Software Development Plan described later in Section 3.2. As illustrated in Figure 1, each team member had a defined role in

overall 4d-Var code development. The portion of the WBS that came under AER's responsibility is included in the original proposal for this project. That SOW is excerpted in Sections 2.3.4.1 to 2.3.4.5 below.

2.3.4.1 Alpha Test Code Build

During this phase, the CHSSI team was charged with further development and improvement of the baseline code to the levels required for Alpha release. AER commenced efforts to develop scalable forward model components of the 4d-Var system. The components are spelled out in the Software Development Plan and are summarized below:

- **Non-linear Forecast Model:** Download and run the most recently available version of the MM5 non-linear model (NLM) in order to familiarize the CWO-5 programming team with the constructs used there to implement scalability. This is the same-source paradigm used in the MM5 NLM to enable parallelization of the executable code while still having one source code for both single and multiprocessor platforms (described in Section 2.3.6). Ensure agreement between output of serial code and parallel codes running both on a single and on multiple processors. Incorporate into the CWO-5 4d-Var system updated versions of the NLM code, as these updates become available.
- **Tangent-linear Forecast Model:** Develop a new TLM based on the release of MM5 used as the NLM. Make use of tangent-linear and adjoint compilers in this effort (described later in Section 2.3.5). Make the tangent-linear model scalable in a manner similar to that used to build the same-source parallel NLM: Incorporate same-source parallel modifications to the executable build structure by adding the FORTRAN Loop and Index Converter (FLIC; http:// www-unix.mcs.anl.gov/~michalak/flic/) and Runtime System Library (RSL; http://www-unix.mcs.anl.gov/~michalak/rsl/) libraries. Perform data decomposition of static data structures. Analyze data dependencies in subroutines and implement inter-processor communication. Adapt I/O, model initialization, and namelist configuration to parallel architecture. Obtain agreement between output of non-parallel code and both parallel code running on a single processor and parallel code running on multiple processor through substantial testing. Conduct performance optimization.
- **Documentation:** Produce initial version of user's guide for alpha testers. Documentation is to include instructions on installation, configuration, execution, and test cases.

The primary AER activity during this development phase consisted of preparing a TLM code based on MM5v3 of the NLM. The TLM modules were then subject to a series of correctness tests. After the TLM passed the correctness tests, the codes were handed over to our NCAR partner for coding changes that would permit scaling on MPP systems. These coding changes implement domain decomposition. To accomplish this our NCAR partner utilized the RSL, which makes calls to the Message Passing Interface

(MPI; http://www-unix.mcs.anl.gov/mpi/) standard and the FLIC. These coding changes were applied to both the NLM and the TLM codes. At this time, the CWO-5 team selected a subset of users to serve as formal Alpha testers and established procedures for monitoring Alpha release and user feedback. When (1) the code consistently satisfied the performance criteria required by the TEMP Addendum, (2) procedures were in place to adequately track code releases and gather user feedback, and (3) the code was running well on at least one DoD HPC platform, we scheduled the Alpha Test Review with the HPCMO program office. The project team provided the CHSSI Project Manager with the necessary documentation and a completed testing checklist at the Alpha test review. During this period, AER served as the Software Configuration Management (SCM) Manager and had the responsibility for ensuring the proper entries were made in the Software Development Library (SDL). This includes generation of documentation, test reports, software, and any other pertinent materials.

2.3.4.2 Beta Test Code Build

After the Alpha Review, the team examined the Alpha code and addressed the functionality and usability issues, identify bugs, inconsistencies, confusing points, etc. These changes are recorded in the history log maintained by the Concurrent Version System (CVS; http://www.cvshome.org/) for each of the 4d-Var modules. At the same time, the development team began planning for new Beta code development activities by integrating new functionality, fixes, as well as changes identified during the Alpha test period. The most notable change was the implementation of the parallel ADJ code by our NCAR team member. During this phase, AER prepared software documentation. When the code achieved "full" functionality on two or more DoD HPC platforms and was in a usable state by the CTA community (Computational Technology Area; in our case Climate/Weather/Oceanography), the team scheduled the Beta test review. The components are spelled out in the Software Development Plan and are summarized below:

- **Non-linear Forecast Model:** Incorporate bug fixes encountered in the Alpha Test Code;
- **Tangent-linear Forecast Model:** Incorporate bug fixes encountered in the Alpha Test Code;
- **Adjoint Model:** Develop a new MM5 adjoint model based upon the latest release of MM5 used as the NLM. Incorporate same-source parallel modifications to the executable build structure by adding the FLIC and RSL libraries. Perform data decomposition of static data structures. Modify loops and index arithmetic to re-establish "Owner Computes" and to eliminate instances of false recursion introduced with the creation of the adjoint model. Make modifications to FLIC to automate code changes in the previous step. Analyze data dependencies in subroutines and implement inter-processor communication. Adapt I/O, model initialization, and namelist configuration to parallel architecture. Obtain agreement between output of non-parallel code and both parallel codes running on a single processor and parallel code running on multiple processor through careful testing. Conduct performance optimization;

- **Raob Observation Operator:** Develop observation operator for radiosonde observations;
- **Satellite Observation Operator:** Develop observation operator for GOES-8 satellite sounder radiances;
- **Documentation:** Produce beta version of user's guide. This version will be comprehensive enough for users not previously familiar with the 4d-Var system to implement it with minimal effort.

During the Beta Test Code build, AER served as the focal point for the Problem/Change Request (P/CR) process outlined in the Software Development Plan (SDP) for any action items that came up during the Alpha Test Review. This would normally involve coordinating changes to both code and the SDL. However, the majority of the effort was directed at optimization of the ADJ of the 4d-Var system. As with the NLM and TLM during Alpha Code Build, the ADJ was also placed under version control (CVS) and configured with the UNIX make and make_mpp utilities. Functions were added to the baseline 4d-Var code that permitted access to and quality control of satellite radiance data that will serve as an important source of data for each analysis. During the Beta Test Code Build AER managed the activities related to the SDL.

2.3.4.3 Initial Operating Code Build

After the Beta test review is concluded, the team released the Beta test version to a broad spectrum of test users for Beta testing, or use in a more application-oriented mode, and provide feedback on any residual errors or functional problems and deficiencies. The CTA and project leaders reviewed the results and lessons learned during the Beta test period and determined what functions and capabilities should go into the final Initial Operating Capability (IOC) "version 1.0" of the CHSSI code. The team added these additional functions, incorporated remaining fixes identified during Beta test, and updated the documentation. When the code and supporting documentation and processes were fully functional on *two or more* HPC platforms and the code was ready for release to the general DoD community, the team will declare itself ready for IOC. The components are spelled out in the Software Development Plan and are summarized below:

- **Non-linear Forecast Model:** Incorporate bug fixes encountered in Beta testing and physics upgrades to the 4d-Var system;
- **Tangent-linear Forecast Model:** Incorporate bug fixes encountered in Beta testing and physics upgrades to the 4d-Var system;
- **Adjoint Model:** Incorporate bug fixes encountered in Beta testing and physics upgrades to the 4d-Var system;
- **Satellite Observation Operator:** Incorporate bug fixes encountered in Beta testing;
- **Documentation:** Enhance of the user's guide based on Beta user's comments.

During the IOC Code Build, AER was responsible for managing any remaining core programming activities related to the adjoint model as well as the P/CR process for any

action items that might arise during the Beta Test Review and Beta test user feedback. AER also continued in its role as SCM Manager for all relevant SDL activities.

2.3.4.4 Data Acquisition and Quality Control

AER was responsible for identifying, obtaining, calibrating and validating required satellite radiance, upper-air and supporting data. Data sources included the Air Force Interactive Meteorological System, and national archive sites maintained by NCAR. AER utilized tools produced in a separate project that performed a quality control step on the GOES-8 sounder data. This data processing step eliminated cloud-contaminated pixels from the data stream and removed the bias between the measured GOES-8 brightness temperatures and those computed from collocated radiosonde data.

2.3.4.5 Systems Engineering and Program Management

AER, in its role as Configuration Manager, provided Configuration Management (CM) services for all aspects of the CHSSI 4d-Var code development. This included CM for the Software and Document Libraries during the development of reusable software and during the development of new software. The components are spelled out in the Software Development Plan and are summarized below:

- **Planning:** Compose the SDP and TEMP Addendum, requirements analysis, outlining the structure of any software that needs to be developed, and periodic adjustment of plans based on how the project is proceeding;
- **Configuration Management:** Set up a consistent CVS code repository. Set up a consistent document repository for controlling all relevant project documents in addition to user documentation. Compose and implement the Configuration Management Plan that contains procedures for the use of the repository. Include policies for the maintenance of the repository over the life of the project;
- **Quarterly and Financial Reporting:** Provide all required CHSSI reporting to the Program Manager. Financial documents were archived in the SDL.

AER provided contractual and other software and documentation releases of the CWO-5 code, following established procedures documented in the AER Quality Management System.

2.3.5 Migration to MM5v3

The current MM5 forecast model is now up to Version 3 (MM5v3) and includes substantial coding and physics upgrades over MM5v1. John Michalakes, our technical consultant, suggested in an email communication after the Software Acceptance Review that rather than introduce changes to the existing MM5v1 4d-Var to make that system scalable, the CWO-5 development team should instead to base its 4d-Var code on MM5v3. This meant that the development team would have to create updated versions of the tangent-linear and adjoint models (TLM and ADJ, respectively) to be compatible with the latest release of the MM5 at that time, Version 3.4. The final decision to update the TLM and ADJ to Version 3 weighed feedback from potential users of the code and issues

related to the maintainability of the code. The structure of the CWO-5 MM5v3 Adjoint Modeling System is illustrated in Figure 2. The green colored boxes refer to codes that required no further updates, otherwise known as "non-development items." The orange colored boxes represent new components of the 4d-Var system that had to be developed and tested for correctness for this project in order to attain consistency with Version 3 of the MM5. The methodology for developing these components is described in Section 3.

After the HPCMO approved this change of work plan, AER produced an updated WBS to reflect the new MM5v3 4d-Var development path and began the software process for the development of new code. We selected a development tool call the Tangent-Adjoint Model Compiler (TAMC; http://www.autodiff.com/tamc/; Geiring and Kaminski 1998). We adopted a hybrid approach for developing new software with TAMC (Figure 3): First, manual changes to the MM5v3 NLM modules eliminated non-standard Fortran 77 code (e.g., POINTER statements). INCLUDE statements were also removed. Then, TAMC generated the TLM and ADJ code. The POINTER and INCLUDE statements were returned to the new modules, which were then ready for testing.

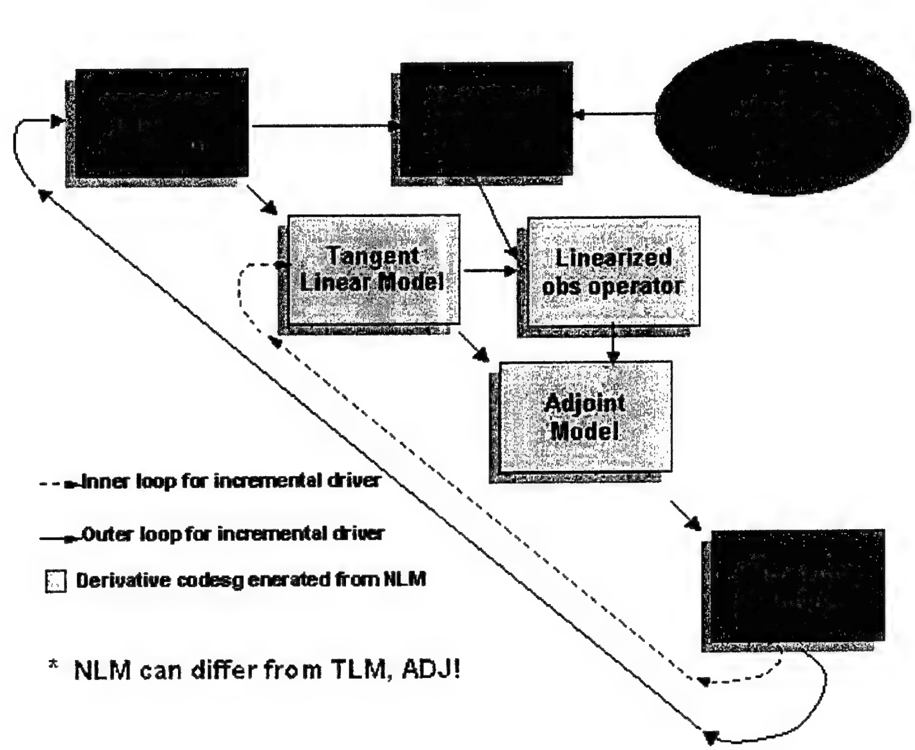

Figure 2. Schematic Diagram of Incremental 4d-Var

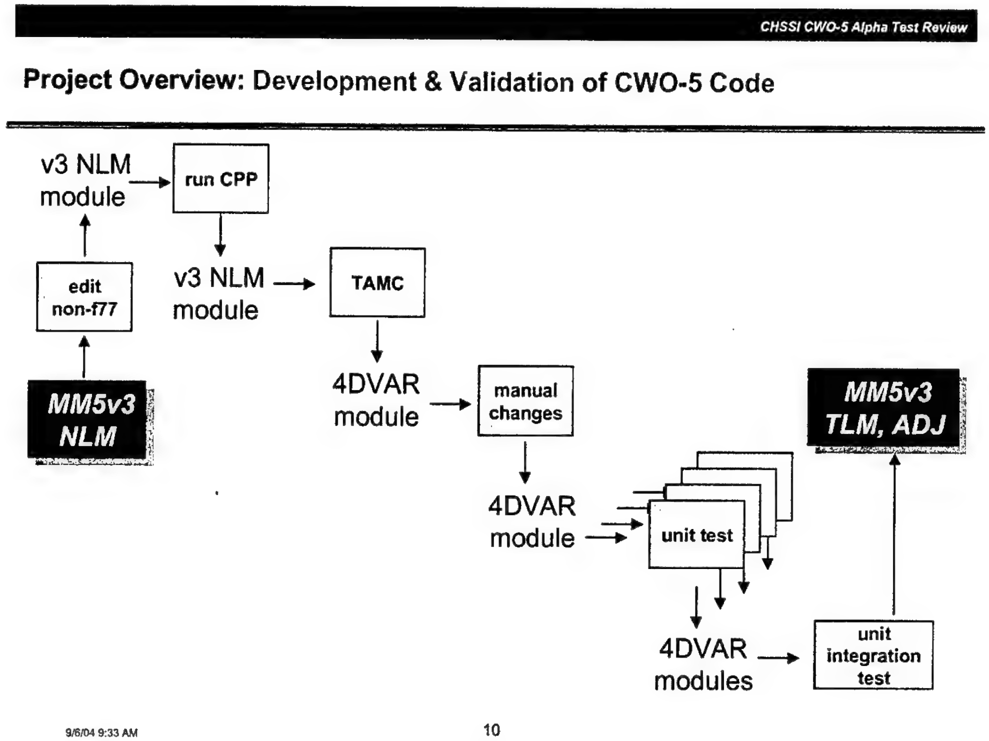

Figure 3. Illustration of Testing Procedure Adopted in CWO-5 TLM and ADJ Code Development

2.3.6 Distributed Memory Architecture Issues

A project of this size introduces a number of important software engineering and programming issues relevant to this project. Fortunately, most of these issues were addressed during the development of the Distributed Memory (DM) version of the MM5 forecast model. These were outlined in a document entitled Introduction to the Distributed Memory-Parallel MM5 System, and another entitled 4d-Var Driver Parallelization Issues.

2.3.7 Funding Structure

AFRL was awarded a CHSSI grant for this project on 2 November 1999. In order to expedite progress on AER tasks and responsibilities outlined in Table 1, AFRL provided some of the initial funding to AER on a previously negotiated contract with AER (F19628-96-C-0053). This allowed AER to begin work on some of the initial documentation requirements soon after AFRL received funding (February 2000). The contract between AER and AFRL negotiated specifically for this project (F19628-00-C-0054) was signed on 8 June 2000.

3. METHODS AND PROCEDURES

3.1 Requirements Analysis

The requirements analysis process develops the basis for the entire project effort. CHSSI project proposals are a first step in this process. They consider how existing codes perform on new HPC platform(s) and where their difficulties/risks have been and will be. From this, project scientists can determine to some level of detail what needs to be done to maximize performance, efficiency, usability, functionality, scalability, portability, etc. This analysis forms the basis of the project proposal, and it can be used to determine many of the project's test requirements later in the process. The requirements analysis determines the project goals, such as "be able to model a 10 million atom problem," or "process 256x256-pixel images at rates up to 45 frames per second to allow real-time analysis." The requirements analysis defines the project's baseline or starting point--the amount of existing code from which you're starting. This baseline provides the HPCMO team with a benchmark against which to measure progress throughout the course of the project.

The general requirement for CWO-5 was to create a scalable version of an existing 4d-Var analysis system that can assimilate satellite radiance data and is computationally efficient enough to run in real-time on a massively parallel processing supercomputer.

3.2 Software Development Plan

Project teams normally spend a considerable amount of time defining what they want to accomplish (their goals) and planning how they will accomplish those goals. A common tool used to record the results of this planning is a Software Development Plan (SDP), which details the major tasks or phases of the total effort, including the test activities used to verify progress as the project is executed. A critical step in the definition of the SDP is to define the functionality envisioned in each version of the code that's developed.

This SDP was developed in conformance with MIL-STD-498 (http://www.software.org/quagmire/descriptions/mil-std-498.asp). [Note that MIL-STD-498 was cancelled in June 1998, when it was superceded by IEEE/EIA 12207.] It is structured in sections following the format and content provisions of Data Item Description (DID) DI-IPSC-81427. Each section identifies tailoring applied to the structure and instructions for content defined in the DID. The structure of the overall CHSSI CWO-5 project procedures is patterned after MIL-STD-1521 (http://sparc.airtime.co.uk/users/wysywig/1521b.htm). [Note that MIL-STD-1521 was cancelled in April 1995, when it was superceded by MIL-STD-973 (http://wwwedms.redstone.army.mil/edrd/973.html).] The general contents of the CWO-5 SDP are described in Table 2.

AER worked with AFRL to complete the CWO-5 SDP.

Table 2. Outline of the CWO-5 Software Development Plan

Section	Description
1	Scope; system and document overviews; relation to other documents
2	Documents referenced by this SDP and used during its preparation
3	Overview of the required work, including work breakdown structure and spend plan
4	Plans for general software development activities
5	Details of all software planning, design, development, reengineering, integration, test, evaluation, Software Configuration Management (SCM), product evaluation, and preparation for delivery activities
6	Defines the project schedule and activity network including year by year deliverables
7	Describes the project organization and the resources required to accomplish the work
8	Contains the acronyms used in the SDP

3.2.1 Software Development Process

The software development plan describes a process to develop software in an incremental series of builds, beginning from a pre-selected reusable software code (i.e., the MM5v1 4d-Var and MM5v3 NLM). The CWO-5 software team developed the 4d-Var system in accordance with processes defined in Section 5 of the SDP in the context of the software engineering process model presented in Figure 4. Note that CHSSI projects generally begin with established codes, i.e., codes that have effectively fulfilled the initial processes shown in Figure 4, including Software Requirements, Preliminary Design, and Detailed Design. The CWO-5 process integrated reusable software from existing sources with newly developed software. Software design and coding was the responsibility of the Software Development Group (generally, AER, NCAR, and FSU) using an object oriented design approach. AER and AFRL defined the Test Case Descriptions, Test Procedures, and conducted the Unit and Unit Integration code tests. AER prepared a Software Test Plan (STP) that described test procedures and next executed test cases defined in the TEMP. These tests generated Software Test Reports (STRs) that described results of both unit and unit integration tests. A record of the activities and results of the software development process were logged in the Software Development Files (SDFs). These files, along with other pertinent project references were deposited and maintained in the SDL and made available to support management reviews, metrics calculations, quality audits, product evaluations, and preparation of product deliverables. All facets of the software engineering process are under configuration management and follow AER's quality management procedures.

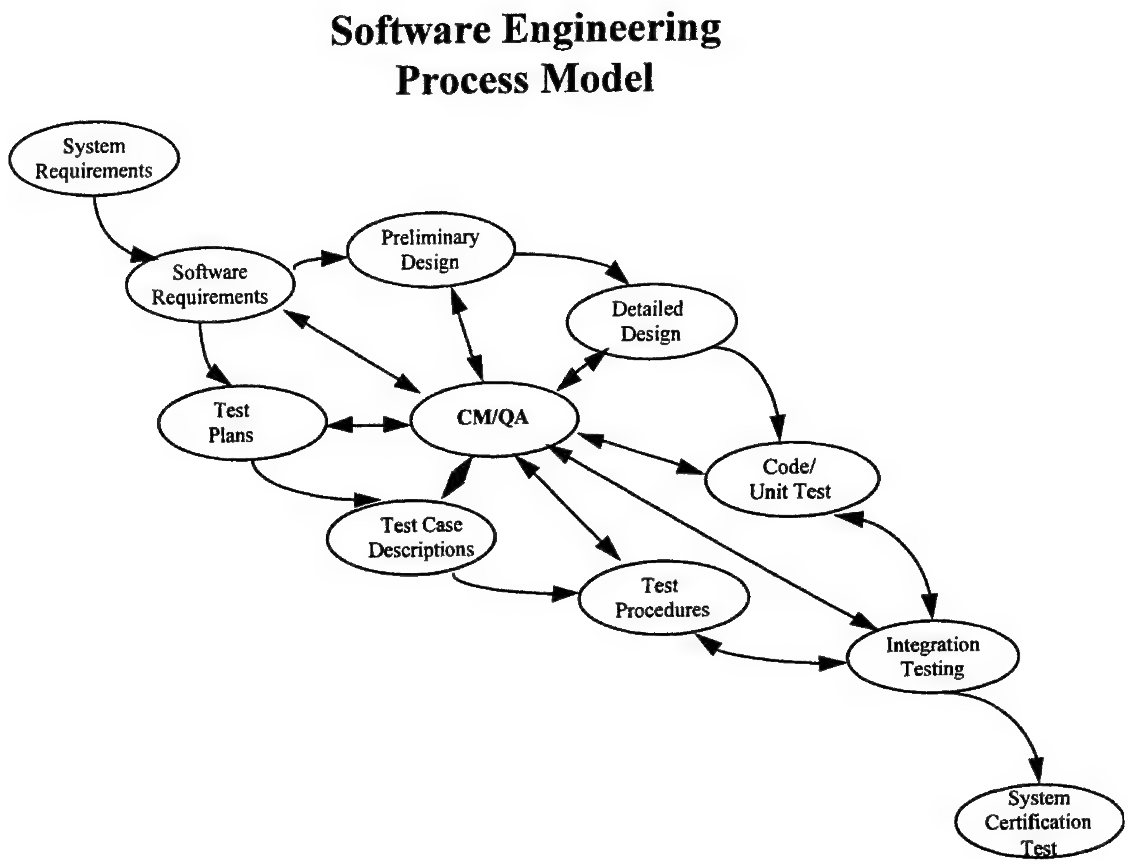

Figure 4. Software Engineering Process Model

3.3 Test and Evaluation Master Plan (Addendum)

As the Software Development Plan is created, the test plan that will verify the success of the development efforts is created as well. Each project's test program is summarized in an addendum to the CHSSI Test and Evaluation Master Plan, or TEMP. The TEMP Addendum contains the Measures of Effectiveness and Suitability (MOE&S), or metrics. The MOE&S's are cross-referenced to the Critical Technical Parameters (CTP) necessary to successfully achieve the MOE&S, and are also cross-referenced to the Critical Operational Issues. The CWO-5 CTPs are shown in Table 3. TEMP Addendum also contains Program Management Indicators that are used to assess the overall performance of AFRL and collaborators and their ability to develop and follow reasonable and appropriate procedures for managing a software effort of this size and scope.

AER and AFRL together created the CWO-5 TEMP Addendum document.

Table 3. Critical Technical Parameters

CRITICAL TECHNICAL PARAMETER	TEST EVENT (SAT, ALPHA, BETA, IOT&E)	OBJECTIVES (Target Values)	THRESHOLDS (Minimum Required Values)	Decision Supported
Scalable software suites	SAT	• Wall-clock time baseline established for single-processor	• Wall-clock time baseline established for single-processor	Full Scale Development
	ALPHA	• Wall-clock time reduced by 32 times that of baseline on non-linear and tangent-linear components	• Wall-clock time reduced by 16 times that of baseline on non-linear and tangent-linear components	Alpha Release
	BETA	• Wall-clock time reduced by 32 times that of baseline for all components	• Wall-clock time reduced by 16 times that of baseline for all components	Beta Release
	IOT&E	• Wall-clock time reduced by 64 times that of baseline for all components	• Wall-clock time reduced by 32 times that of baseline for all components	Milestone III
Portable application software	SAT	• Codes will run on one HPC platforms producing valid results	• Codes will run on one HPC platform producing valid results	Full Scale Development
	ALPHA	• Codes will run on two HPC platforms with same valid results	• Codes will run on two HPC platforms with same valid results	Alpha Release
	BETA	• Codes will run on three HPC platforms with same valid results	• Codes will run on two HPC platforms with same valid results	Beta Release
	IOT&E	• Codes will run on three or more HPC platforms with same valid results	• Codes will run on two HPC platforms with same valid results	Milestone III

Table 3 (Cont'd)

CRITICAL TECHNICAL PARAMETER	TEST EVENT (SAT, ALPHA, BETA, IOT&E)	OBJECTIVES (Target Values)	THRESHOLDS (Minimum Required Values)	Decision Supported
Correctness	SAT	• At least 1 analysis from test case produces accurate, valid output	• At least 1 analysis from test case produces accurate, valid output	Full Scale Development
	ALPHA	• At least 2 analyses from test case produce accurate, valid output	• At least 1 analysis from test case suite produce accurate, valid output	Alpha Release
	BETA	• At least 3 analyses from test case produce accurate, valid output	• At least 2 analyses from test case produce accurate, valid output	Beta Release
	IOT&E	• Three or more sub-problems from test case suite produce accurate, valid output; satellite data improves RMSE in forecasts of analysis dependent-variables	• At least 3 sub-problems from test case suite produce accurate, valid output; satellite data improves RMSE in forecasts of analysis dependent-variables	Milestone III
Correctness	SAT	• Output on multiprocessor machine runs agrees with single-processor vector-class benchmark results to within 5%	• Output on multi-processor machine runs agrees with single-processor vector-class benchmark results to within 10%	Full Scale Development
	ALPHA	• Output from multi-processor runs agrees with single-processor results to within 1%	• Output from multi-processor runs agrees with single-processor results to within 5%	Alpha Release
	BETA	• Output from multi-processor runs agrees with single-processor results to within numerical round-off error	• Output from multi-processor runs agrees with single-processor results to within 1%	Beta Release
	IOT&E	• Output from multi-processor runs agrees with single-processor results exactly	• Output from multi-processor runs agrees with single-processor results to within numerical floating-point round-off	Milestone III

3.4 Software Acceptance Test Review

Once the SDP is approved and the code is developed to the point that it has achieved some initial minimum performance levels, it is preferable to hold a Software Acceptance Test (SAT) review--the first major technical milestone for the project. The

SAT is a review of the scope, plan, problems, direction, "state-of-the-code," etc. for each effort. At the review, the major questions are "Is it a sound project with a reasonable chance of success?", "Does is have an acceptable level of risk?", "Do we know where we want to go and how to get there?", and "Will the project provide enough added HPC capability to the DoD to make it worth the money?" SAT reviews are held once the size and scope of a project is determined and the feasibility of applying a project to HPC technology can be discussed. The CWO-5 SAT review was held about 6 months into the project, on 29 June 2000. The SAT decision authority is the CTA leader; the formal decision at SAT is whether to proceed with HPC parallel software development. If the project is approved, the project team then begins the Alpha phase of development.

The HPCMO requested certain pre-review material, which the CWO-5 team provided. Next, the CWO-5 team outlined the action items it felt were necessary in order to be prepared for the SAT. The CWO-5 SAT was held 29 June, 2000 at AFRL on Hanscom AFB, MA. The HPCMO forwarded its approval for CWO-5 to proceed to Alpha testing on 6 July, 2000.

3.5 Alpha Test Code Review

The Alpha test review is the second major milestone on CHSSI projects. It is typically held 15 to 18 months into a 3-year project. The chairman of the Alpha test review is the CTA leader. At the Alpha test review, an independent panel (panel members can be members of the HPCMO staff or a reviewer external to the project) evaluates the code(s) against the test criteria, reviews the project's internal procedures and external interfaces, and provides recommendations to the chairman. The approval authority for Alpha pass/fail is the CHSSI Project Manager. The decision at Alpha is whether the code should be released to a "friendly" set of users to provide their impressions of the code's functionality and usability. The project team will provide the CHSSI Project Manager a set of documentation and the completed testing checklist at the Alpha test review.

If the project is approved to continue, the test users wring out the Alpha code functionality and usability, identify bugs, inconsistencies, confusing points, etc. At the same time, the development team begins the Beta code development activities by integrating new functionality, fixes, and changes identified during the Alpha test period and incorporated into the production version of the code. During this phase, the project team also prepares thorough software documentation. When the code has achieved "full" functionality on two or more DoD HPC platforms and is in a usable state by the CTA community, the team will schedule the Beta test review.

The Alpha Test Review for CWO-5 took place on 5 November, 2001 at AFRL on Hanscom AFB, MA. In advance of the review, the CWO-5 team put together a plan to address all outstanding issues. The plan maps the requirements to a series of tasks that the CWO-5 team had to complete to pass the review. The CWO-5 team prepared a post-review report to document the results of the review activities. After approval from the HPCMO, an Alpha Release was assembled and made available to Alpha testers. Results of the Alpha Review and Alpha Release are discussed in Section 4.1.

3.6 NCAR Release

The success of the CHSSI program is judged, in part, by the number of scientists and researchers who benefit from the scalable codes that are produced by the projects. In the case of CWO-5, our primary focus was on AFWA; however, we also wished for the wider meteorological community to benefit from this project. The CWO-5 team felt that if the CWO-5 4d-Var application were approved as part of the MM5 release software, the code would attain a legitimacy beyond what we could otherwise achieve. The CWO-5 project team approached NCAR with this idea. NCAR agreed to do this, and the team delivered a "non-CHSSI" release to NCAR for acceptance testing. The release contains user documentation, a registration form, and the CWO-5 code and test data.

The NCAR release was similar to the Alpha Test Code release in that it was not yet fully scalable, so testing at NCAR was confined to correctness tests of the serial version. However, the NCAR release did include bug fixes to the Alpha code. Some additional bugs were discovered during NCAR's acceptance testing, and incorporated into the Beta Test Code.

3.7 Beta Test Code Review

The Beta test review is the third major project milestone. It is typically held 6-12 months after the Alpha test review, or about 30 months into a 3-year project. An independent test team is again used to review the Beta version of the code and the documentation prepared. These items are compared to the criteria set forth in the TEMP Addendum. The team also reviews the lessons learned and procedures used during the previous Alpha testing period. The review panel for Beta test review consists at a minimum of the CTA leader and a representative from the HPCMO. The CWO-5 review panel included representation from NCAR. The decisions at Beta are whether the code is ready for IOT&E and whether to release the formal Beta version of the code. The approval authority for Beta pass/fail is the CHSSI Project Manager. The Beta Test Code usually includes a set of documentation and the completed testing checklist.

The TEMP Addendum Critical Test Parameters for the Beta Review were collected and packaged in a form suitable to the HPCMO. The HPCMO received the CWO-5 Beta test results in a report from the Program Manager. The Beta Test Review for CWO-5 was held on 18 September 2002 at the offices of the HPCMO in Alexandria, VA.

After the Beta test review concluded, the team released the Beta Test Code to a broad spectrum of test users and provided feedback on any residual errors or functional problems and deficiencies. The CTA and project leaders reviewed the results and lessons learned during the Beta test period and determined what functions and capabilities should go into the final Initial Operating Capability (IOC) "version 1.0" of the CHSSI code. The team added these additional functions, incorporated remaining fixes identified during Beta test, and updated the documentation. When the code and supporting documentation and processes were fully functional on three or more HPC platforms and the code is ready for release to the general DoD community, the team declares itself ready for IOC. Results of the Beta Test Code Review and Beta Test Code Release are discussed in Section 4.2.

3.8 Initial Operational Capability Version

The initial guidance from the HPCMO indicated there would be an IOT&E review. However, the HPCMO later clarified to the CWO-5 Program Manager that the Beta Test Code would be the last reviewable release. After satisfactory completion of any Beta test review action items, the CTA leader submits a memorandum to the CHSSI Project Manager certifying closure of the action items, certifying completion of proper documentation and supporting procedures, and indicating successful closure of the project. The approval authority for IOT&E pass/fail is the HPCMO. Following approval, the IOC software is released to the full user community for operational testing and use. The features included in the IOC version are the observation operator for GOES-8 satellite radiance assimilation, the tropical cyclone bogus data assimilation, the incremental driver, and upgraded physics parameterizations for the TLM and ADJ.

One of the obstacles to operational implementation of 4d-Var algorithms is their large computational cost. Compared to 3d-Var, each iteration of the minimization procedure contains an additional calculation of the nonlinear forecast model and its adjoint. Even with the speedups gained through parallelization of the MM5 4d-Var in the CWO-5 CHSSI project, this cost is prohibitive for most, if not all, current MM5 forecast applications at AFWA. A variant of the 4d-Var algorithm, named "incremental 4d-Var," was proposed by Courtier *et al.* (1994), which provides for significant speedups in the minimization procedure. The operational implementation of 4d-Var at the ECMWF makes use of the incremental formulation. In terms of the unified notation of Ide *et al.* (1997), the minimization for the incremental 4d-Var takes the form

$$J[\delta\mathbf{x}(t_0)] = \frac{1}{2}\{\delta\mathbf{x}(t_0) - [\mathbf{x}^{\mathrm{b}}(t_0) - \mathbf{x}^{\mathrm{g}}(t_0)]\}^{\mathrm{T}} \mathbf{B}_0^{-1} \{\delta\mathbf{x}(t_0) - [\mathbf{x}^{\mathrm{b}}(t_0) - \mathbf{x}^{\mathrm{g}}(t_0)]\}$$

$$+\frac{1}{2}\sum_{i=0}^{n}[\mathbf{H}_i\delta\mathbf{x}(t_i) - \mathbf{d}_i]^{\mathrm{T}}\mathbf{R}_i^{-1}[\mathbf{H}_i\delta\mathbf{x}(t_i) - \mathbf{d}_i], \tag{3}$$

where the increment is defined as $\delta\mathbf{x}(t_0) = \mathbf{x}(t_0) - \mathbf{x}^{\mathrm{g}}(t_0)$. The TLM, which is linearized about the NLM forecast from the guess $\mathbf{x}^{\mathrm{g}}(t_0)$, is used to predict values of $\delta\mathbf{x}(t)$; similarly, a linearized version of the observation operator is used in the evaluation of (3). The solution to the minimization problem, $\delta\mathbf{x}^{a}(t_0)$, is used to obtain an updated value of $\mathbf{x}^{\mathrm{g}}(t_0)$, and nonlinear effects are incorporated through performing this procedure in a number of outer iterations. A schematic of this process is shown in Figure 2. Further approximations are usually made by using simplified dynamics in the linearized model and its adjoint, and/or by using decreased resolution (or smaller spectral truncation), in the inner loop. Formally, this can be written in terms of a linear simplification operator from $\delta(\mathbf{x})$ to a subset of gridpoints (or, spectral modes), $\delta\mathbf{w}$.

Additional features that were to be incorporated by FSU into the IOC version are the Bogus Vortex Data Assimilation (BDA) and upgraded physics parameterizations. The BDA scheme was developed by FSU and incorporated into a later release of the CWO-5

code. It permits the use of bogus data to initialize a tropical cyclone vortex (see, e.g., Zou and Xiao 2000). Additional physics parameterizations were the Grell (1993) cumulus convection and the simple microphysics parameterization described by Dudhia (1989).

3.9 4d-Var Document Repository

Documentation for the CWO-5 Alpha and Beta Test Code releases are available on the software distribution disk. Each provides information on the background of the CWO-5 4d-Var application, installation, building and executing the code, and advanced options such as making modifications and testing. The distribution disk also includes documentation that was prepared for the MM5v1 4d-Var application, and a general description of adjoint techniques. The software distribution disk is available from AER. Inc.

3.10 4d-Var Code Repository

The guidance provided by the HPCMO at the beginning of CWO-5 indicated that the development processes defined for each CHSSI project should "mirror" Level 2 of the Software Engineering Institute's (SEI) Capability Maturity Model (http://www.sei.cmu.edu/cmm/). Formal software development practices usually require some sort of version control procedures. For CWO-5, we implemented version control with CVS. The CWO-5 CVS repository resides on a computer at the offices of AER, Inc. in Lexington, MA. An export of this repository is included on the distribution disk. Instructions on using the CWO-5 4d-Var are included in the software delivery component of this contract.

3.11 Optical Turbulence Task

Funding to support AER, Inc.'s participation in the HEL-JTO project became available in March 2002. AER, Inc. hosted a kickoff meeting with our AFRL HEL-JTO project manager and technical POC (Frank Ruggiero) on 26 April 2002. At that time, Dr. Ruggiero provided AER with a copy of PL-TR-93-2043, "A Model for (Optical Turbulence) Profiles Using Radiosonde Data" by Dewan et al. (1993) as well as an introductory slide presentation of the HEL program, goals, and objectives. Note that after the sensitivity and uncertainty analyses were complete, the HEL-JTO funding situation changed so that we were unable to proceed with the C_n^2 observation operator and 4d-Var data assimilation studies.

AER supported the AFRL's HEL-JTO project through the development, test, and evaluation of an observation operator for C_n^2. We first outlined a technical approach for the task. AFRL used the MM5 forecast model system to provide input for the C_n^2 model and produce forecasts of optical turbulence. The forecasts were then compared to observations from a thermosonde database. This task investigated the potential utility of C_n^2 data as a data *source* that could be assimilated with the CWO-5 4d-Var application. The objective would be to improve the quality of the initial lower stratospheric analysis by incorporating the additional information that the thermosondes could provide. Before we could do this, we thought it would be wise first to explore the potential benefit of

thermosonde data assimilation through a series of analyses. As a result, the optical turbulence task consisted of four sub-tasks:

3.11.1 Sensitivity Analysis

The C_n^2 model described in Dewan et al. (1993) uses information about the dynamic and thermal structure of the atmosphere. The structure is described by multiple parameters of the MM5 forecast model. When using the variational method with a forecast system like MM5, one must be able to transform the model dependent variables into the observed quantity. Knowing the sensitivity of C_n^2 to the MM5 model will be useful in understanding how well suited this data source will be for data assimilation. We conducted an adjoint sensitivity analysis of the optical turbulence profile with respect to profiles of the atmospheric (or, MM5) variables of state (u, v, T, P). The sensitivity analysis was patterned after the one outlined by Xiao and Zou (2001) for the GOES-8 radiance observation operator. The analysis computes the relative sensitivity, or fractional change of a response function to a given fractional change of a model input,

$$\left(\frac{\nabla J \delta \mathbf{x}}{J}\right) \Big/ \frac{\delta x}{x} \tag{4}$$

where J is the response function, ∇J is the output of the adjoint, and δx is a perturbation vector.

3.11.2 Uncertainty Analysis

It will be useful to understand how the errors in the MM5 model inputs translate into errors in the C_n^2 profiles. The error covariance matrices in (1) determine those structures in the background and observations that ought to be weighted less heavily than others. In this subtask we estimate the linear propagation of errors through the C_n^2 observation operator. The method uses the TLM and ADJ of a forecast model to predict forecast error variances from an initial estimate of the analysis error variance. From this the analysis will provide guidance on the potential for the C_n^2 data to have a positive impact on the analysis.

3.11.3 Observation Operator

If the uncertainty analysis in Section 3.11.2 shows that the C_n^2 data contains information that would be beneficial to an analysis, then it might be advantageous to proceed with the development of a C_n^2 observation operator that would relate the model state to optical turbulence. This would require that we modularize the Dewan model code for use in the MM5v3 4d-Var system and eventual data assimilation studies, and test the operator.

3.11.4 Data Assimilation Studies

With the C_n^2 observation operator developed and tested as described in Section 3.11.3, we can then proceed to do 4d-Var data assimilation studies of C_n^2, where the impact of the optical turbulence data is measured in some controlled way.

4. RESULTS AND DISCUSSION

The results of the CWO-5 project were demonstrated during a series of reviews. These results are summarized below. Material of more interest to the general meteorological community was presented at several conferences. (See Nehrkorn et al. 2001a, Nehrkorn et al. 2001b, Ruggiero et al. 2001).

4.1 Alpha Test Review

The CWO-5 team successfully passed the Alpha Test Review. The Critical Test Parameters for the Alpha Review and the CWO-5 results are presented in Table 4. We conducted tests with the scalable TLM and the serial 4d-Var applications. Other materials included with the test materials are the test drivers and results for the TLM and 4d-Var unit integration tests, the Alpha Test Code Users' Document, and the CWO-5 internal test plan and test report presented to the HPCMO. At the time of the Alpha Test Review, the CWO-5 4d-Var code was not yet completely scalable; the ADJ code was still undergoing test and evaluation. In order to show conformance with the CTP for speedup, we conducted tests with the TLM portion of the CWO-5 code. During the speedup testing, we discovered that I/O was the main impediment to speedup. The parallel file system in use on the test IBM SP computer system was not optimally handling the parallel I/O. Our NCAR partner (John Michalakes) determined that buffering the NLM output and the TLM input caused a marked increase in the speedup of the parallel system. Other techniques were limiting the read/write operations to the local sub domain, and using asynchronous reads and writes. This problem/change process had the benefit of being applicable to later development of the parallel ADJ. At the time of the Alpha Test Review, the CWO-5 code could run on 2 HPC platforms (SGI Origin and IBM SP-3). The serial 4d-Var code results (i.e., gradient) agreed to within 13 digits. The CWO-5 code was also run on 2 different cases at the time of the Alpha Review. The results of the serial and MPP version of the TLM driver test differed by less than 1 percent. These results are available in detail in the Alpha Review presentation in the test materials file on the distribution disk.

Table 4. Critical Test Parameters (CTPs), the Tested Values and Test Result, and the Objective and Threshold Requirements for the CWO-5 Alpha Test Review

CTP	Tested Value & Test Result	Evaluation Optimum Objectives	Evaluation Minimum Threshold
Scalable software suites • Demonstrate wall-clock time speed-up as a function of increased Central Processing Units (CPU)	Tested Value: 20.9(TLM) 19.7(NLM) Test Result: ___Fails to meet Minimum Threshold X__Meets Minimum Threshold ___Meets Optimum Objective	• Wall-clock time reduced by 32 times that of baseline on non-linear and tangent-linear components	• Wall-clock time reduced by 16 times that of baseline on non-linear and tangent-linear components
Portable application software • Software application functions the same and produce similar results, within an acceptable margin of error, on a variety of scalable HPC platforms.	Tested Value: 2 Test Result: ___Fails to meet Minimum Threshold ___Meets Minimum Threshold X__Meets Optimum Objective	• Codes will run on two HPC platforms with same valid results	• Codes will run on two HPC platforms with same valid results
Correctness: • Run software on multiple analyses and compare with results of baseline code	Tested Value: 2 Test Result: ___Fails to meet Minimum Threshold ___Meets Minimum Threshold X__Meets Optimum Objective	• At least 2 analyses from test case produce accurate, valid output	• At least 1 analysis from test case suite produce accurate, valid output
Correctness: • Insure results from MPP runs agree with single processor runs	Tested Value: 0% Test Result: ___Fails to meet Minimum Threshold ___Meets Minimum Threshold X__Meets Optimum Objective	• Output from multi-processor runs agrees with single-processor results to within 1%	• Output from multi-processor runs agrees with single-processor results to within 5%

4.2 Beta Test Review

The Beta Test Review was held on 18 September, 2002 at the offices of the HPCMO in Alexandria, VA. The Critical Test Parameters for the Beta Review and the CWO-5 results are presented in Table 5. We conducted tests with the scalable 4d-Var application, which, unlike the Alpha Test Code, contained the scalable ADJ. Other materials included with the test materials are the test results for the 4d-Var unit integration tests, the Beta Test Code Users' Document, and the CWO-5 internal test plan and test report presented to the HPCMO. Lessons learned during the Alpha phase of the project helped to produce impressive levels of speedup in the 4d-Var application. Our NCAR partner (John Michalakes) determined that buffering the NLM output and the TLM input caused a marked increase in the speedup of the parallel system. Other techniques were limiting the read/write operations to the local sub domain, and using asynchronous reads and writes. This problem/change process had the benefit of being applicable to later development of the parallel ADJ. At the time of the Alpha Test Review, the CWO-5 code could run on 2 HPC platforms (SGI Origin and IBM SP-3). The serial 4d-Var code results (i.e., gradient) agreed to within 13 digits. The CWO-5 code was also run on 2 different cases at the time of the Alpha Review. The results of the serial and MPP version of the TLM driver test differed by less than 1 percent. The log of the overall TLM test and development was maintained in the TLM Software Development File.

The GOES-8 observation operator was developed and tested with the MM5v3 4d-Var system. Some results from a simple test case are presented below. The GOES-8 domain from which the test data was selected is shown in Figure 5. Note on this particular day there was a large amount of cloud cover. Since only data from cloud-free areas could be used, the amount of data actually selected for assimilation was relatively small. Figure 6 shows the temperature difference at two model levels between the Aviation Model analysis (AVN) and the CWO-5 4d-Var data assimilation that included GOES-8 infrared sounding data. Figure 7 is the same as Figure 6, but for moisture. Note that the largest effect is over the relatively cloud-free region near southern Georgia.

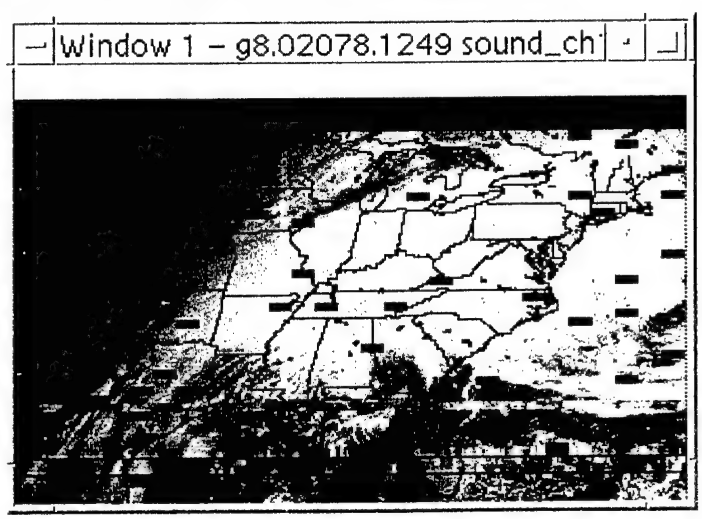

Figure 5. Visible-Band Data from GOES-8 Sounder Channel 19 for 1249 UTC on 19 March 2003. Black Rectangles Represent Regions of Missing Data.

Table 5. Critical Test Parameters (Ctps), the Tested Values and Test Result, and the Objective and Threshold Requirements for the CWO-5 Beta Review

Critical Technical Parameter	Evaluation Optimum Objectives	Evaluation Minimum Threshold	Tested Value and Test Result		
			IBM SP3	SGI Origin 3000	Compaq ES-45
Scalable Software Suites	Wall-clock time reduced by 32 times that of baseline for all components	Wall-clock time reduced by 16 times that of baseline for all components	**Tested Value:** 55 – SESAME case 28 – Iniki Case **Test Result:** ___Fails to meet Minimum Threshold _X_ Meets Minimum Threshold ___Meets Optimum Objective	**Tested Value:** No Test **Test Result:** ___ Fails to meet Minimum Threshold ___Meets Minimum Threshold ___Meets Optimum Objective	**Tested Value:** 196 – SESAME case 76 – Iniki case **Test Result:** ___ Fails to meet Minimum Threshold ___Meets Minimum Threshold _X_ Meets Optimum Objective
Portable Application Software	Codes run on three HPC platforms with same valid results	Codes run on two HPC platforms with same valid results	**Tested Value:** 2 cases run with valid results **Test Result:** ___ Fails to meet Minimum Threshold _X_ Meets Minimum Threshold ___Meets Optimum Objective	**Tested Value:** No Test **Test Result:** ___ Fails to meet Minimum Threshold ___Meets Minimum Threshold ___Meets Optimum Objective	**Tested Value:** 2 cases run with valid results **Test Result:** ___ Fails to meet Minimum Threshold _X_ Meets Minimum Threshold ___Meets Optimum Objective

Table 5 (Cont'd)

Critical Technical Parameter	Evaluation Optimum Objectives	Evaluation Minimum Threshold	Tested Value and Test Result		
			IBM SP3	**SGI Origin 3000**	**Compaq ES-45**
Correctness	At least 3 analyses from test cases produce accurate, valid output	At least 2 analyses from test cases produce accurate, valid output	**Tested Value:** 2 cases run with valid results **Test Result:** ___ Fails to meet Minimum Threshold _X_ Meets Minimum Threshold ___ Meets Optimum Objective	**Tested Value:** No Test **Test Result:** ___ Fails to meet Minimum Threshold ___ Meets Minimum Threshold ___ Meets Optimum Objective	**Tested Value:** 2 cases run with valid results **Test Result:** ___ Fails to meet Minimum Threshold _X_ Meets Minimum Threshold ___ Meets Optimum Objective
Correctness	Output from mult-processor runs agrees with single-processor runs to within numerical round-off error	Output from mult-processor runs agrees with single-processor runs to within 1%	**Tested Value:** < 0.02% **Test Result:** ___ Fails to meet Minimum Threshold _X_ Meets Minimum Threshold ___ Meets Optimum Objective	**Tested Value:** No Test **Test Result:** ___ Fails to meet Minimum Threshold ___ Meets Minimum Threshold ___ Meets Optimum Objective	**Tested Value:** < 0.26% **Test Result:** ___ Fails to meet Minimum Threshold _X_ Meets Minimum Threshold ___ Meets Optimum Objective

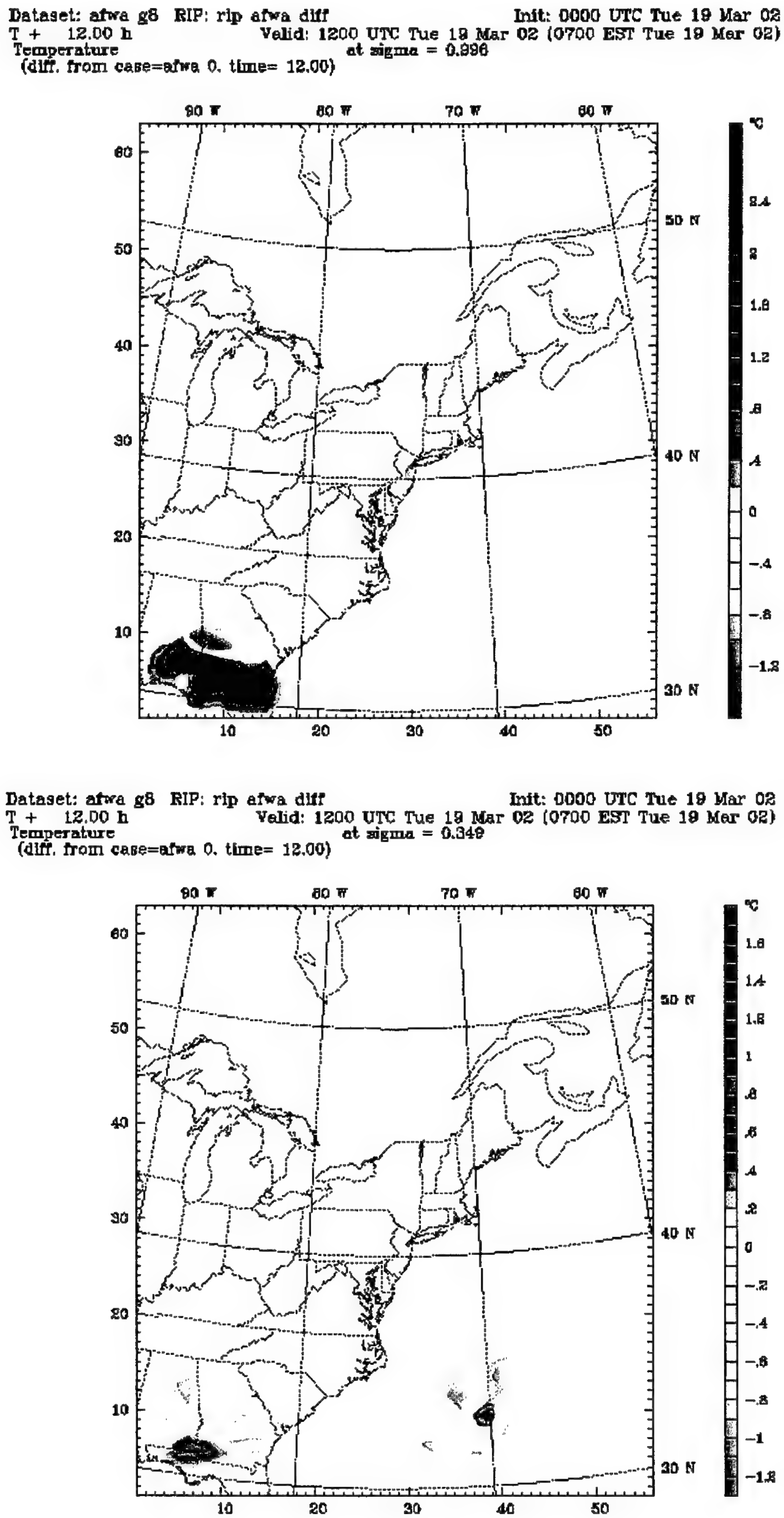

Figure 6. Temperature Difference (C) Between AVN and MM5v3 4d-Var Analyses Valid 12 UTC 19 March 2003 for σ=0.996 (top) and σ=0.349 (bottom).

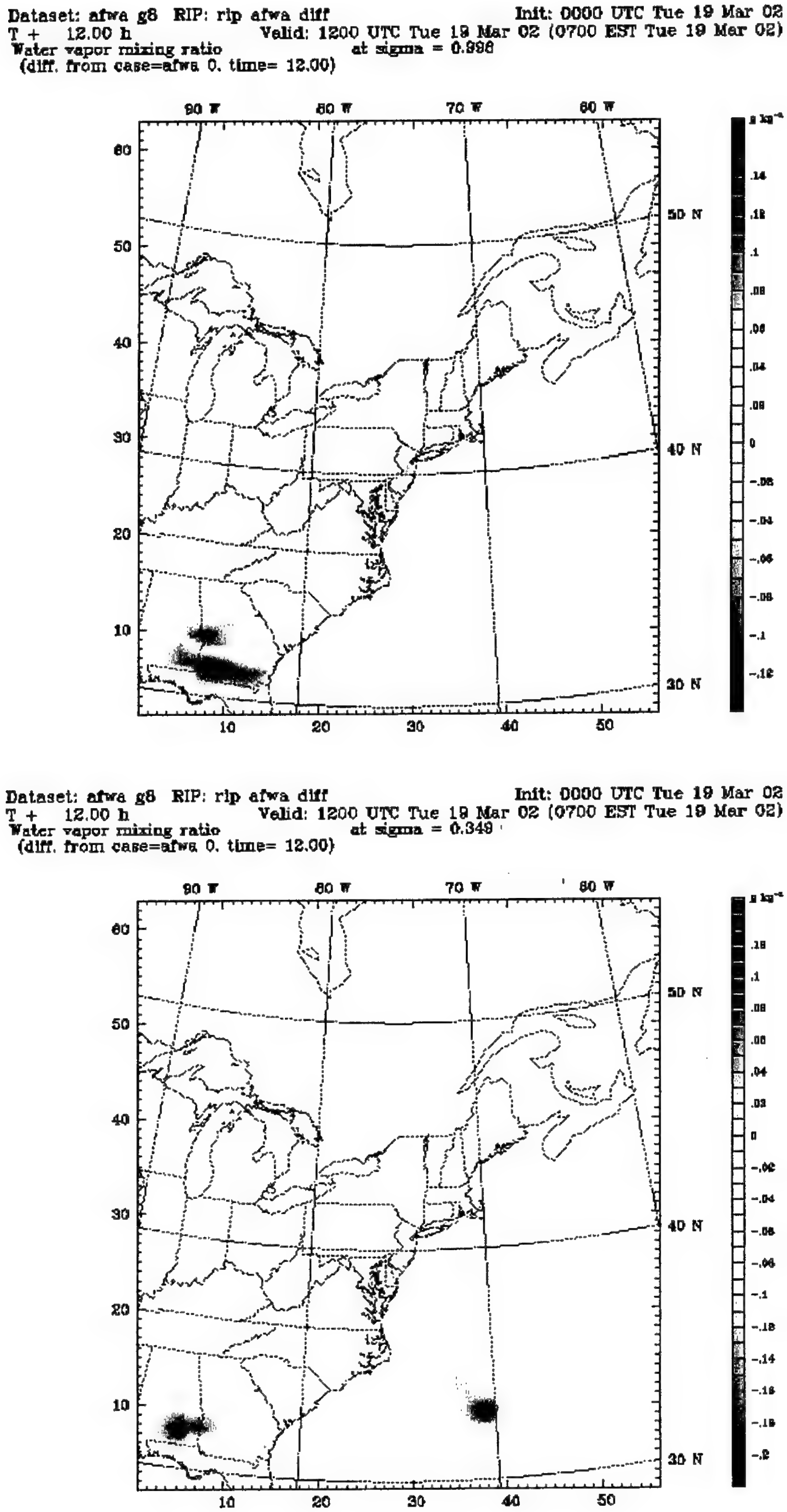

Figure 7. Same as Fig. 6, but for Water Vapor Mixing Ratio (gkg^{-1})

4.3 Optical Turbulence Task

We conducted a study to develop an optical turbulence observation operator that could potentially improve forecasts of C_n^2 for the Air Force. The study first explored the suitability of the C_n^2 data for data assimilation in a system like the MM5v3 4d-Var. Two questions we wanted to answer before we attempted the data assimilation were "How sensitive is the modeled C_n^2 quantity to the input MM5 variables?" and "What is the uncertainty of the observed C_n^2 compared to that from the MM5 model?"

We were provided by AFRL a thermosonde dataset collected at Vandenberg AFB, CA during the period 18-25 October 2001. We compared the C_n^2 data directly observed by the thermosonde to that computed from radiosonde values of u, v, T, and p (the thermosonde and radiosonde were on the same balloon). We began with an accepted model of C_n^2 (Dewan et al. 1993). The object was to see how well correlated directly observed C_n^2 was to the values computed by the C_n^2 model. The correlation ranged from 0.84 to 0.49 with an average correlation of 0.69. An example is shown in Figure 8. The correlation for this particular time (02 UTC) was 0.75.

Having an idea on the upper limit of how well the C_n^2 model fit the data, we next focused on the sensitivity and uncertainty tests. For this we derived the TLM and ADJ. The sensitivity analysis revealed greatest C_n^2 sensitivity to temperature perturbations below 15-km to u-wind speed above 10-km. A plot of the sensitivity of C_n^2 to the model variables is given in Figure 9. Plots for the other time levels of data are qualitatively similar (not shown).

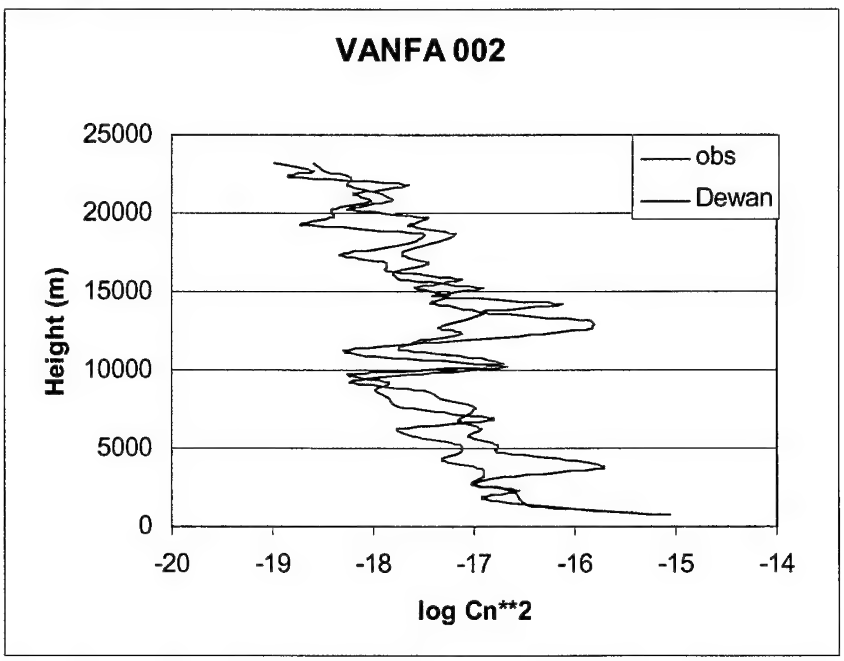

Figure 8. Observed C_n^2 Thermosonde Data from Vandenberg AFB, CA vs. C_n^2 Derived from MM5 Forecast Model Output Valid at the Same Time. Correlation = 0.75

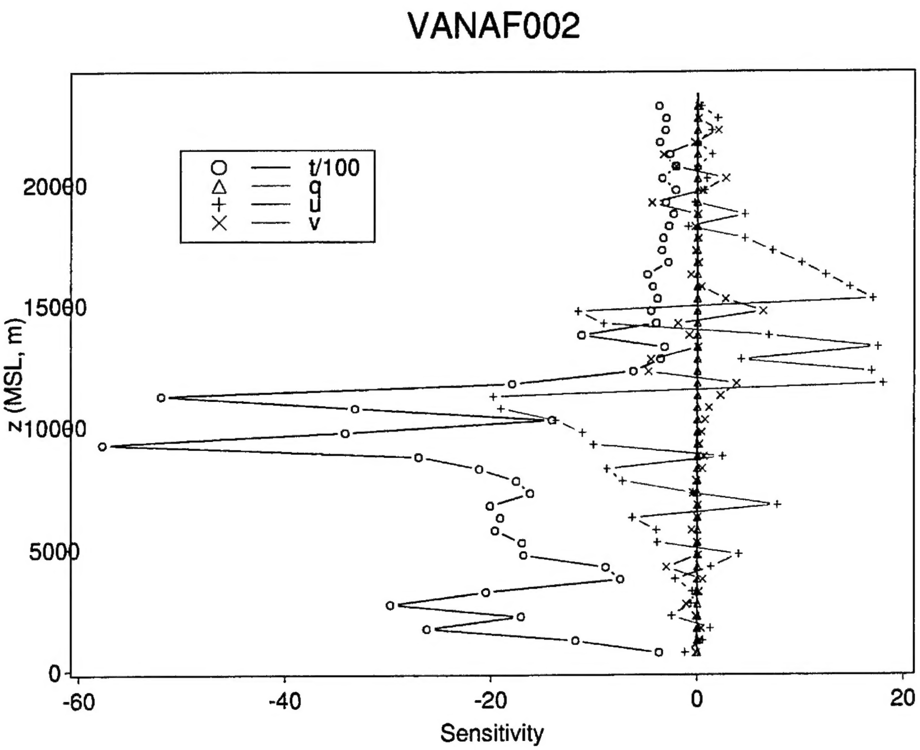

Figure 9. Sensitivity of C_n^2 as a Function of Height to Perturbations in Wind (u, v), Temperature (T), and Moisture (q)

The uncertainty analysis attempts to estimate the linear propagation of errors through the observation operator. When this error (uncertainty) is quantified, it can be compared to the observed C_n^2 error; if the observed C_n^2 errors are smaller than the modeled C_n^2 (the observed data is "better" than the modeled data), then we can presume that the introduction of observed data (e.g., from a data assimilation system) will improve the analysis of variables in the modeling system. An example of this comparison is illustrated in Figure 10. In this figure, the uncertainty in the C_n^2 observations is represented by the spread of computed C_n^2 for different models of the optical turbulence parameter. The dominant contribution to the observation error is the uncertainty in the forward model. The modeled uncertainty is represented by error bars and is overlaid on the C_n^2 model plots. The plot suggests that for this case from 5 to 15-km above ground level, we should expect a measurable improvement in the analysis, since the simulated C_n^2 error (due to the NWP model forecast error) is larger than the uncertainty in the observation.

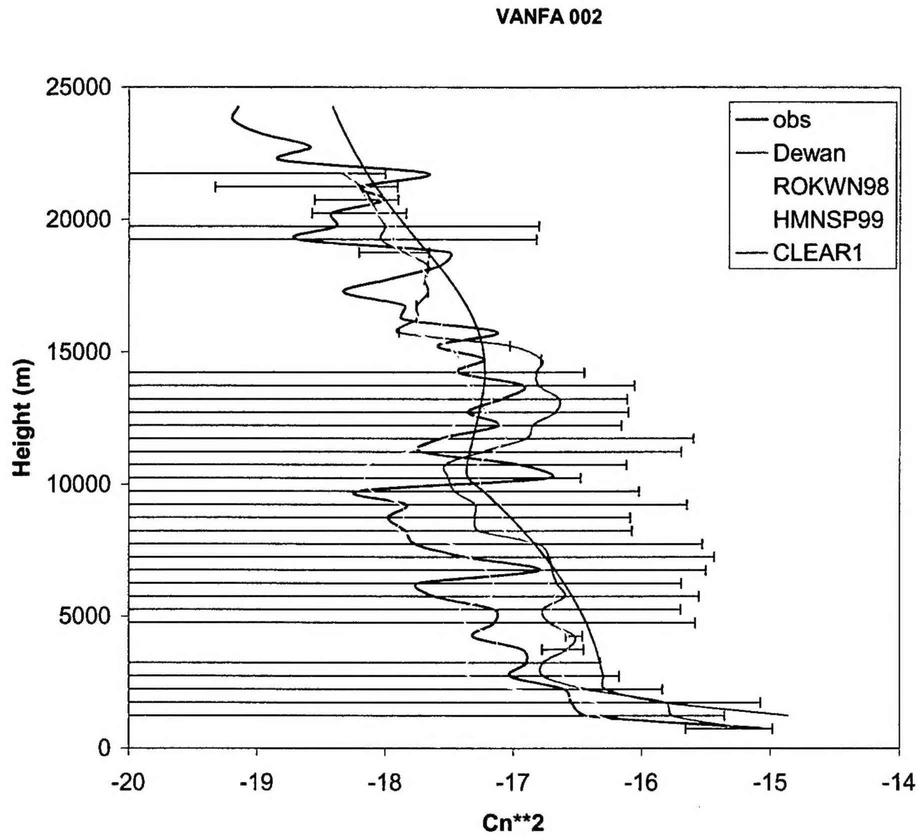

Figure 10. Uncertainty Analysis Showing Relative Error of the Various C_n^2 Models and Model State Error Bars. The Information Content In The C_n^2 Data Will Reduce the Uncertainty in Those Regions Where the Spread of the C_n^2 Models is *Less* Than the Width of the Error Bars. (For Error Magnitudes That Exceed the Forecast Values of C_n^2, the Error Bar Extends to Negative Infinity on the Logarithmic Scale.)

As stated in Section 3.11, our original plan included the development of an optical turbulence observation operator and integration and testing of the operator in the CWO-5 4d-Var system. Due to a loss of funds from the High Energy Laser/Joint Technology Office, which originally supported this optical turbulence task, we had to end our studies after the data suitability task described in this section. Therefore, we were not able to develop and test the C_n^2 observation operator.

5. CONCLUSIONS

The work conducted for this contract was primarily directed toward supporting the AFRL CWO-5 CHSSI project. That project was focused on the development and testing of a scalable version of the MM5 4d-Var application. At the start of the project, the 4d-Var code was based on version 1 of the MM5. Following established software development procedures and after consideration of numerous factors, the CWO-5 development team updated the MM5 4d-Var code to version 3. This necessitated the

development and test of a new code for the MM5v3 TLM and ADJ. The CWO-5 code successfully passed the Alpha and Beta Test Reviews. The CWO-5 code was distributed to numerous Alpha and Beta test users and has been used extensively in R&D projects at AER, including projects for DoD clients. Additional studies examined the impact of optical turbulence parameter (i.e., C_n^2) assimilation. The preliminary results from that study suggest that C_n^2 data have the potential to improve upper-atmospheric analyses and the NWP model forecasts made from them when integrated within a data assimilation framework, such as the 4d-Var method.

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